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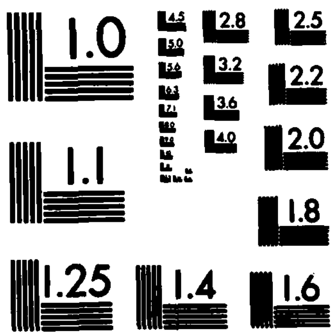

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SUPPLEMENTARY NOTES

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19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

We have studied a number of computational problems in numerical linear algebra. Most of these problems arise in statistical computations. They include the following: (1) Application of the conjugate gradient method to nonorthogonal analysis of variance; (2) Use of orthogonalization procedures in geodetic problems; (3) Algorithms for computing sample variance; (4) Truncated Newton methods; (5) Imposing Curvature Restrictions on Flexible Functional Forms.

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2. FOREWORD

In this project, we have tackled a number of matrix problems which have wide applicability. For very large sets of data, it is necessary to perform numerical calculations so that the investigator can have confidence in the numberical results. Furthermore, it is desirable to perform the computation in an efficient manner, even when powerful computers are used. We have attempted to devise methods which satisfy the properties of efficiency and accuracy.

3. NOT APPLICABLE

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5. a. Statement of the Problem Studied and
   b. Summary of the Most Important Results

Below are abstracts of the papers published under this grant.

"Large-Scale Geodetic Least-Squares Adjustment by Dissection and Orthogonal Decomposition," by Gene H. Golub and Robert J. Plemmons. Abstract: Very large-scale matrix problems currently arise in the context of accurately computing the coordinates of points on the surface of the earth. Here geodesists adjust the approximate values of these coordinates by computing least-squares solutions to large sparse systems of equations which result from relating the coordinates to certain observations such as distances or angles between points. The purpose of this paper is to suggest an alternative to the formation and solution of the normal equations for these least-squares adjustment problems. In particular, it is shown how a block-orthogonal decomposition method can be used in conjunction with a nested dissection scheme to produce an algorithm for solving such problems which combines efficient data management with numerical stability. The approach given here parallels somewhat the development of the natural factor formulation, by Argyris et al., for the use of orthogonal decomposition procedures in the finite-element analysis of structures. As an indication of the magnitude that these least-squares adjustment problems can sometimes attain, the forthcoming readjustment of the North American Datum in 1983 by the National Geodetic

Survey is discussed. Here it becomes necessary to linearize and solve an overdetermined system of approximately 6,000,000 equations in 400,000 unknowns - a truly large scale matrix problem.

"Truncated Newton Methods," by Stephen G. Nash. Abstract: The problem of minimizing a real-valued function F of n variables arises in many contexts. Most methods for solving this problem have their roots in Newton's method, i.e. they are based on approximating F by a quadratic function Q. If the number of variables n is large, then Newton's method can be problematic since it requires the computation and storage of the Hessian matrix of second derivatives. Use of finite-differencing and sparse-matrix techniques has overcome some of these problems but not all.

In this thesis, we examine a flexible class of methods, called truncated-Newton methods. They are based on approximately minimizing the quadratic function Q using an iterative scheme such as the linear conjugate-gradient algorithm. A truncated-Newton algorithm is made up of two sub-algorithms: an outer non-linear algorithm controlling the entire minimization, and an inner linear algorithm for approximately minimizing Q.

The most important choice is the selection of the inner algorithm. When the Hessian matrix is known to be positive-definite everywhere, then the basis linear conjugate-gradient algorithm can be used. If not, Q may not have a minimum. We have used the correspondence between the linear conjugate-gradient algorithm and the

Lanczos algorithm for tridiagonalizing a symmetric matrix to develop methods for the indefinite case.

The performance of the inner algorithm can be greatly improved through the use of preconditioning strategies. Preconditionings can be developed using either the outer nonlinear algorithm or using information computed during the inner algorithm. A number of diagonal and tridiagonal preconditioning strategies are derived here.

Numerical tests show that a carefully chosen truncated-Newton method can perform significantly better than the best non-linear conjugate-gradient algorithms available today. This is important since the two classes of methods have comparable storage and operation counts, and they are the only methods available for solving many large-scale problems.

"Algorithms for computing the sample variance: analysis and recommendations," by Tony F. Chan, Gene H. Golub, and Randall J. LeVeque. Abstract: The problem of computing the variance of a sample of N data points (x_i) may be difficult for certain data sets, particularly when N is large and the variance is small. We present a survey of possible algorithms and their round-off error bounds, including some new analysis for computations with shifted data. Experimental results confirm these bounds and illustrate the dangers of some algorithms. Specific recommendations are made as to which algorithm should be used in various contexts.

"Nonorthogonal analysis of variance using a generalized conjugate-gradient algorithm," by Gene H. Golub and Stephen G. Nash. <u>Abstract</u>: A method is developed that computes an exact nonorthogonal analysis of variance using cell means. The method is iterative and does not require that the non-orthogonal design matrix be stored or formed. At each stage in the process, a balanced analysis of variance problem must be solved. A monotonicity property for the estimates of the regression sum of squares is derived that could be used to minimize iteration in hypothesis testing. An application of the algorithm to the solution of analysis of covariance problems is also given.

"Imposing curvature restrictions on flexible functional forms," by A. Ronald Gallant and Gene H. Golub. <u>Abstract</u>: A general computational method for estimating the parameters of a flexible functional form subject to convexity, quasi-convexity, concavity, or quasi-concavity at a point, at several points, or over a region are set forth and illustrated with an example.

Gram-Schmidt Orthogonalization. Long experience of using Gram-Schmidt has given some insights into the behavior of that algorithm, and a manuscript was submitted for publication. These two problems are studied: first, what happens when nonorthogonal vectors are used in the process, and second, how orthogonalization in elliptic norms and by oblique projectors should be done.

Gram-Schmidt orthogonalization is a crucial part of several eigenvalue algorithms. For the Arnoldi method, a basis of the Krylov space is orthogonalized, and in other algorithms it is important that the residual is orthogonal to an appropriately chosen subspace. (Axel Ruhe)

Rational Krylov Sequences. This is a starting point for the development of an entirely new class of algorithms for eigenvalue problems. The algorithms that are now most successful use vectors from a Krylov subspace, which has the powers of the matrix as a basis and thus yields polynomials. Algorithms are being studied which are based on rational functions of the matrix (computed by shifting and inverting). These ideas have been discussed in seminars, but neither experimental results nor written reports are available yet.

It is conceivable that a similar concept is usable for computing matrix functions, and a possible application to ODE solvers has been discussed with Prof. Germund Dahlquist. (Axel Ruhe)

Toda lattice methods for eigenvalue computation.

A method which replaces an eigenvalue problem by a set of ordinary differential equations, and proceeds by applying an ODE solver to those, has been proposed by Prof. Deift et al at New York University. That algorithm has been tested; also, a few variants which involve shifting and inversion have been developed. The experiments hitherto showed that, though innocent-looking, the system needs many steps of an ODE solver in order to reach the solution. An interesting fact is that the number of steps barely grows with n, the order of the matrix, but it is doubtful whether there are any problems where it really performs better than e.g. QR. On the other hand, by tracking its progress documented by plots, one gains insights that are of value to understand the behavior of tridiagonal eigenproblems, and possibly get assistance in developing other algorithms. (Axel Ruhe)

5. c. Publications and Technical Reports

"Large-Scale Geodetic Least-Squares Adjustment by Dissection and Orthogonal Decomposition," by Gene H. Golub and Robert J. Plemmons, _Linear Algebra and its Applications_ 34:3-27 (1980).

"Truncated-Newton Methods," by Stephen G. Nash, Ph.D. dissertation, Stanford University, May 1982

"Algorithms for Computing the Sample Variance: Analysis and Recommendations," by Tony F. Chan, Gene H. Golub, and Randall J. LeVeque, Technical Report #22, Yale University, Dept. of Computer Science. To be published in _J. American Statistical Assoc._

"Nonorthogonal Analysis of Variance Using a Generalized Conjugate-Gradient Algorithm," by Gene H. Golub and Stephen G. Nash, Journal of the American Statistical Assoc., March 1982.

"Imposing Curvature Restrictions on Flexible Functional Forms," by A. Ronald Gallant and Gene H. Golub, Discussion Paper #538, North Carolina State University, November 1982

5.d. Scientific Personnel:

Gene H. Golub, Principal Investigator

John Hershberger

Mark Lake

Axel Ruhe

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